# Nuclear recoil corrections to the $2p_{\frac{3}{2}}$ state energy of hydrogen-like and high $Z$ lithium-like atoms in all orders in $\alpha Z$

A.N.Artemyev, V.M.Shabaev, and V.A.Yerokhin

*Department of Physics, St.Petersburg State University, Oulianovskaya 1, Petrodvorets, St.Petersburg 198904, Russia*

Nuclear recoil corrections ...

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**Abstract**

The relativistic nuclear recoil corrections to the energy of the $2p_{\frac{3}{2}}$ state of hydrogen-like and the $(1s)^2 2p_{\frac{3}{2}}$ state of high $Z$ lithium-like atoms in all orders in $\alpha Z$ are calculated. The calculations are carried out using the B-spline method for the Dirac equation. For low $Z$ the results of the calculation are in good agreement with the $\alpha Z$ -expansion results. It is found that the total nuclear recoil contribution to the energy of the $(1s)^2 2p_{\frac{3}{2}} - (1s)^2 2s$ transition in lithium-like uranium constitutes $-0.09\,eV$.

# 1 Introduction

Till recently accurate QED calculations of the nuclear recoil corrections to atomic energy levels were of interest mainly in connection with high precision measurements of the Lamb shift in hydrogen [1,2]. In this case the nuclear recoil corrections may be calculated in lowest orders in $\alpha Z$ ($\alpha$ is the fine structure constant, $Z$ is the nuclear charge). However recent achievements in experimental investigations of highly charged ions [3] require calculations of the nuclear recoil corrections right up $Z = 92$. In the last case the parameter $\alpha Z$ can no longer be considered small and, so, the calculations without expansion in $\alpha Z$ are required.

In our previous paper [4] we calculated the nuclear recoil corrections in all orders in $\alpha Z$ for the $1s$, $2s$, $2p_{\frac{1}{2}}$ states of hydrogen-like atoms and the $(1s)^2 2s$, $(1s)^2 2p_{\frac{1}{2}}$ states of high $Z$ lithium-like atoms. We found that the nuclear recoil contribution to the energy of the $(1s)^2 2p_{\frac{1}{2}}$ - $(1s)^2 2s$ transition in lithium-like uranium constitutes $-0.07\,eV$ and, so, is comparable with the uncertainty of the experimental value of the transition energy: $280.59(10)\,eV$ [3]. We found also the nuclear recoil contribution, additional to Salpeter's one, to the Lamb shift ($n = 2$) of hydrogen to be $-1.32(6)\,kHz$. This result is in good agreement with recent analytical calculations of the $\frac{m^2}{M}(\alpha Z)^6 \ln(\alpha Z)$ and $\frac{m^2}{M}(\alpha Z)^6$ corrections [5-8], according to which the terms of order $\frac{m^2}{M}(\alpha Z)^6 \ln(\alpha Z)$ cancel each other [5,6], the contribution of order $\frac{m^2}{M}(\alpha Z)^6$ is $-0.77\,kHz$ for the $2s$ state [7] and $0.58\,kHz$ for the $2p_{\frac{1}{2}}$ state [8].

In the present paper we extend the results of [4] to the case of the $2p_{\frac{3}{2}}$ state of hydrogen-like and high $Z$ lithium-like atoms.

The relativistic units $\hbar = c = 1$ are used in the paper.

# 2 Hydrogen-like atoms

The complete $\alpha Z$-dependence expressions for the nuclear recoil corrections to the energy levels of hydrogen-like atoms were first derived by one of the authors of the present paper [9] (a part of the expressions was found earlier by Braun [10]). These expressions consist of three contributions: the Coulomb contribution, the one-transverse-photon contribution, and the two-transverse-photon contribution. For a state $a$ the Coulomb contribution is

given by

$$\Delta E_c = \Delta E_c^{(1)} + \Delta E_c^{(2)} , \tag{1}$$

$$\Delta E_c^{(1)} = \langle a|\frac{\mathbf{p}^2}{2M}|a\rangle , \tag{2}$$

$$\Delta E_c^{(2)} = \frac{2\pi i}{M}\int_{-\infty}^{\infty} d\omega\, \delta_+^2(\omega)\langle a|[\mathbf{p},V_c]G(\omega+\varepsilon_a)[\mathbf{p},V_c]|a\rangle , \tag{3}$$

where $|a\rangle$ is the unperturbed state of the Dirac electron in the Coulomb field of the nucleus, $V_c = -\frac{\alpha Z}{r}$ is the Coulomb potential of the nucleus, $\mathbf{p}$ is the momentum operator, $\delta_+(\omega) = \frac{i}{2\pi}(\omega+i0)^{-1}$, $G(\omega) = (\omega - H(1-i0))^{-1}$ is the relativistic Coulomb Green function, $H = \boldsymbol{\alpha}\mathbf{p} + \beta m + V_c$. The one-transverse-photon contribution is

$$\Delta E_{tr(1)} = \Delta E_{tr(1)}^{(1)} + \Delta E_{tr(1)}^{(2)} , \tag{4}$$

$$\Delta E_{tr(1)}^{(1)} = -\frac{1}{2M}\langle a|\Big(\mathbf{D}(0)\mathbf{p} + \mathbf{p}\mathbf{D}(0)\Big)|a\rangle , \tag{5}$$

$$\Delta E_{tr(1)}^{(2)} = -\frac{1}{M}\int_{-\infty}^{\infty} d\omega\, \delta_+(\omega)\langle a|\Big([\mathbf{p},V_c]G(\omega+\varepsilon_a)\mathbf{D}(\omega) - \mathbf{D}(\omega)G(\omega+\varepsilon_a)[\mathbf{p},V_c]\Big)|a\rangle , \tag{6}$$

where

$$D_m(\omega) = -4\pi\alpha Z\alpha_l D_{lm}(\omega) , \tag{7}$$

$\alpha_l$ ($l = 1,2,3$) are the Dirac matrices, $D_{lm}(\omega)$ is the transverse part of the photon propagator in the Coulomb gauge. In the coordinate representation it is

$$D_{ik}(\omega,\mathbf{r}) = -\frac{1}{4\pi}\Big\{\frac{\exp(i|\omega|r)}{r}\delta_{ik} + \nabla_i\nabla_k\frac{(\exp(i|\omega|r)-1)}{\omega^2 r}\Big\} . \tag{8}$$

The two-transverse-photon contribution is

$$\Delta E_{tr(2)} = \frac{i}{2\pi M}\int_{-\infty}^{\infty} d\omega\, \langle a|\mathbf{D}(\omega)G(\omega+\varepsilon_a)\mathbf{D}(\omega)|a\rangle . \tag{9}$$

The terms $\Delta E_c^{(1)}$ and $\Delta E_{tr(1)}^{(1)}$ are leading at low $Z$. These terms can easily be calculated by using the virial relations for the Dirac equation [11-13]. Such a calculation gives [9]

$$\Delta E^{(1)} \equiv \Delta E_c^{(1)} + \Delta E_{tr(1)}^{(1)} = \frac{m^2 - \varepsilon_a^2}{2M}\,. \tag{10}$$

The $\alpha Z$-expansion of this term is given in [4].

The terms $\Delta E_c^{(2)}$, $\Delta E_{tr(1)}^{(2)}$, and $\Delta E_{tr(2)}$ are given in the form that allows one to use the relativistic Coulomb Green function for their calculation. (As was found by Pachucki and Grotch [7], this form is convenient for the $\alpha Z$-expansion calculations as well.) In [4] we transformed these equations to the form that is more convenient for calculations using the finite basis set methods [14] and calculated them for the $1s$, $2s$, and $2p_{\frac{1}{2}}$ states by using the B-spline method for the Dirac equation [15,16]. The calculation for the $2p_{\frac{3}{2}}$ state considered here was carried out in the same way.

Table 1 shows the results of the numerical calculation for the $2p_{\frac{3}{2}}$ state expressed in terms of the function $P(\alpha Z)$ defined by

$$\Delta E^{(2)} = \Delta E_c^{(2)} + \Delta E_{tr(1)}^{(2)} + \Delta E_{tr(2)} = \frac{m}{M}\frac{(\alpha Z)^5}{\pi n^3} P(\alpha Z) mc^2 \tag{11}$$

The functions $P_c$, $P_{tr(1)}$, and $P_{tr(2)}$ correspond to the contributions $\Delta E_c^{(2)}$, $\Delta E_{tr(1)}^{(2)}$, and $\Delta E_{tr(2)}$, respectively. For comparison, the Salpeter's contribution [17] is

$$P_S(\alpha Z) = \frac{8}{3}\,0.030017 - \frac{7}{18} = -0.30884\,. \tag{12}$$

The uncertainties given in the table correspond only to errors of the numerical calculation. In addition, there is an uncertainty due to deviation from the point single particle model of the nucleus used here.

To make a more detailed comparison with the $\alpha Z$-expansion calculations we represent the function $P(\alpha Z)$ in the form

$$P(\alpha Z) = a_1 + a_2 \alpha Z + a_3 (\alpha Z)^2 + a_4 (\alpha Z)^3 \tag{13}$$

The coefficients $a_i$ can be calculated from our numerical results for the $P(\alpha Z)$-function. Such a calculation using the values of the $P(\alpha Z)$-function for $Z$ =1,2,3,5,10,15 gives

$$a_1 = -0.30883, \qquad a_2 = 1.040. \tag{14}$$

The coefficient $a_1$ is in good agreement with the Salpeter's result given by the equation (12). The coefficient $a_2$ coincides, within errors of the numerical procedure, with the corresponding coefficient ($a_2 = 1.047$) obtained by Golosov et.al. [8] ( the related coefficient from the contribution (10) is equal to zero).

According to our numerical calculations the contribution of the difference between $\Delta E^{(2)}$ and Salpeter's correction for the $2p_{\frac{3}{2}}$ state of hydrogen constitutes $0.42(2)\,kHz$. Analytical result for the $\frac{m^2}{M}(\alpha Z)^6$ correction found in [8] gives $0.423\,kHz$. ( In addition to this correction, in [8] the correction of order $\frac{m^2}{M}\alpha^2(\alpha Z)^4$ is calculated to be $0.014\,kHz$.)

Let us consider the nuclear recoil corrections for hydrogen-like uranium. According to the formula (10) the first correction is

$$\Delta E^{(1)}_{2p_{\frac{3}{2}}} = 0.0664\,eV\,. \tag{15}$$

The second correction defined by (11) is

$$\Delta E^{(2)}_{2p_{\frac{3}{2}}} = 0.0014\,eV\,. \tag{16}$$

In the next section we use these results to find the total nuclear recoil contribution to the energy of the $2p_{\frac{3}{2}} - 2s$ transition in lithium-like uranium.

# 3 High Z lithium-like atoms

The complete $\alpha Z$-dependence expressions for the nuclear recoil corrections to the energy levels of high $Z$ few-electron atoms were derived in [18]. These corrections are the sum of one- and two-electron contributions. The one-electron corrections are obtained by summing all the one-electron contributions over all the one-electron states that are occupied. The two-electron corrections for the case considered here are

$$\Delta E^{(int)}_{c} = -\frac{1}{M}\sum_{\varepsilon_n=\varepsilon_{1s}} \langle a|\mathbf{p}|n\rangle\langle n|\mathbf{p}|a\rangle\,, \tag{17}$$

$$\Delta E^{(int)}_{tr(1)} = \frac{1}{M}\sum_{\varepsilon_n=\varepsilon_{1s}} \Big\{\langle a|\mathbf{p}|n\rangle\langle n|\mathbf{D}(\varepsilon_a-\varepsilon_n)|a\rangle + \langle a|\mathbf{D}(\varepsilon_a-\varepsilon_n)|n\rangle\langle n|\mathbf{p}|a\rangle\Big\}\,, \tag{18}$$

$$\Delta E^{(int)}_{tr(2)} \;=\; -\frac{1}{M}\sum_{\varepsilon_n=\varepsilon_{1s}} \langle a|\mathbf{D}(\varepsilon_a-\varepsilon_n)|n\rangle\langle n|\mathbf{D}(\varepsilon_a-\varepsilon_n)|a\rangle\,. \qquad (19)$$

The table 2 shows the results of the calculation of the corrections (17),(18), and (19) for the $(1s)^2 2p_{\frac{3}{2}}$ state expressed in terms of the function $Q(\alpha Z)$ defined by

$$\Delta E^{int} \equiv \Delta E^{(int)}_{c} + \Delta E^{(int)}_{tr(1)} + \Delta E^{(int)}_{tr(2)} = -\frac{2^9}{3^8}\frac{m^2}{M}(\alpha Z)^2 Q(\alpha Z)\,. \qquad (20)$$

Here we have taken into account the known non-relativistic limit of this correction [19]. Within the $\frac{m^2}{M}(\alpha Z)^4$ approximation the function $Q(\alpha Z)$ that we denote by $Q_L(\alpha Z)$ is [20]

$$Q_L(\alpha Z) \;=\; 1+(\alpha Z)^2\Big(-\frac{13}{48}+\frac{1}{2}\ln\frac{27}{32}\Big)\,. \qquad (21)$$

For comparison, this function is given in the table as well. The functions $Q_c(\alpha Z)$, $Q_{tr(1)}(\alpha Z)$, and $Q_{tr(2)}(\alpha Z)$ correspond to the corrections $\Delta E^{(int)}_{c}$, $\Delta E^{(int)}_{tr(1)}$, and $\Delta E^{(int)}_{tr(2)}$, respectively. In leading orders in $\alpha Z$ they are

$$Q_c(\alpha Z) \;=\; 1+(\alpha Z)^2\Big(\frac{17}{48}+\frac{1}{2}\ln\frac{27}{32}\Big)\,, \qquad (22)$$

$$Q_{tr(1)}(\alpha Z) \;=\; \frac{5}{8}(\alpha Z)^2\,, \qquad (23)$$

$$Q_{tr(2)}(\alpha Z) \;=\; -\frac{25}{256}(\alpha Z)^4\,. \qquad (24)$$

For low $Z$, in addition to the corrections considered here, the Coulomb electron-electron interaction corrections to the non-relativistic nuclear recoil contribution must be calculated separately. The main contribution from these corrections is of order $\frac{1}{Z}(\alpha Z)^2\frac{m^2}{M}$.

Let us find the total nuclear recoil contribution to the energy of the $(1s)^2 2p_{\frac{3}{2}} - (1s)^2 2s$ transition in lithium-like uranium. According to our calculation the term $\Delta E^{int}$ contributes $-0.0345\,eV$. Adding to this value the one-electron contribution defined by (15) and (16) and using the related values for the $2s$ state from [4] we find

$$\Delta E_{(1s)^2 2p_{\frac{3}{2}}} - \Delta E_{(1s)^2 2s} = -0.094\,eV.$$

This value is significant enough to be included in accurate QED calculations of the transition energy.

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Table 1: The results of the numerical calculation of the one-electron nuclear recoil corrections to the $2p_{\frac{3}{2}}$ state energy expressed in terms of the function $P(\alpha Z)$ defined by equation (11).

| $Z$ | $P_c(\alpha Z)$ | $P_{tr(1)}(\alpha Z)$ | $P_{tr(2)}(\alpha Z)$ | $P(\alpha Z)$ |
|---|---|---|---|---|
| 1 | 0.0000 | -0.1385(2) | -0.1630(3) | -0.3013(4) |
| 5 | -0.0001 | -0.1230 | -0.1493(1) | -0.2724(1) |
| 10 | -0.0004 | -0.1037 | -0.1338 | -0.2379 |
| 15 | -0.0008 | -0.0841 | -0.1198 | -0.2047 |
| 20 | -0.0012 | -0.0644 | -0.1069 | -0.1726 |
| 25 | -0.0017 | -0.0446 | -0.0950 | -0.1413 |
| 30 | -0.0021 | -0.0245 | -0.0841 | -0.1107 |
| 35 | -0.0026 | -0.0042 | -0.0741 | -0.0081 |
| 40 | -0.0031 | 0.0163 | -0.0649 | -0.0517 |
| 45 | -0.0035 | 0.0372 | -0.0567 | -0.0230 |
| 50 | -0.0040 | 0.0585 | -0.0496 | 0.0050 |
| 55 | -0.0044 | 0.0802 | -0.0432 | 0.0326 |
| 60 | -0.0049 | 0.1025 | -0.0379 | 0.0597 |
| 65 | -0.0054 | 0.1254 | -0.0337 | 0.0863 |
| 70 | -0.0058 | 0.1490 | -0.0307 | 0.1125 |
| 75 | -0.0063 | 0.1735 | -0.0289 | 0.1384 |
| 80 | -0.0068 | 0.1990 | -0.0285 | 0.1638 |
| 85 | -0.0072 | 0.2256 | -0.0294 | 0.1889 |
| 90 | -0.0078 | 0.2534 | -0.0319 | 0.2138 |
| 92 | -0.0080 | 0.2649 | -0.0334 | 0.2236 |
| 95 | -0.0083 | 0.2827 | -0.0361 | 0.2383 |
| 100 | -0.0088 | 0.3135 | -0.0422 | 0.2625 |

Table 2: The results of the numerical calculation of the nuclear recoil correction $\Delta E^{(int)}$ for the $(1s)^2 2p_{\frac{3}{2}}$ state of lithium-like ions expressed in terms of the function $Q(\alpha Z)$ defined by equation (20). $Q_L(\alpha Z)$ is the leading contribution defined by equation (21).

| $Z$ | $Q_c(\alpha Z)$ | $Q_{tr(1)}(\alpha Z)$ | $Q_{tr(2)}(\alpha Z)$ | $Q(\alpha Z)$ | $Q_L(\alpha Z)$ |
|---|---|---|---|---|---|
| 5 | 1.00036 | -0.00083 | 0.00000 | 0.99953 | 0.99953 |
| 10 | 1.00143 | -0.00333 | 0.00000 | 0.99810 | 0.99811 |
| 15 | 1.00323 | -0.00748 | 0.00001 | 0.99573 | 0.99574 |
| 20 | 1.00574 | -0.01330 | 0.00004 | 0.99239 | 0.99242 |
| 25 | 1.00896 | -0.02077 | 0.00010 | 0.98809 | 0.98816 |
| 30 | 1.01291 | -0.02989 | 0.00021 | 0.98281 | 0.98295 |
| 35 | 1.01757 | -0.04065 | 0.00039 | 0.97653 | 0.97679 |
| 40 | 1.02294 | -0.05303 | 0.00065 | 0.96926 | 0.96969 |
| 45 | 1.02902 | -0.06704 | 0.00101 | 0.96097 | 0.96163 |
| 50 | 1.03579 | -0.08264 | 0.00150 | 0.95165 | 0.95264 |
| 55 | 1.04323 | -0.09981 | 0.00212 | 0.94129 | 0.94269 |
| 60 | 1.05132 | -0.11854 | 0.00289 | 0.92988 | 0.93179 |
| 65 | 1.06001 | -0.13877 | 0.00382 | 0.91742 | 0.91995 |
| 70 | 1.06925 | -0.16047 | 0.00488 | 0.90390 | 0.90716 |
| 75 | 1.07894 | -0.18356 | 0.00608 | 0.88930 | 0.89343 |
| 80 | 1.08897 | -0.20796 | 0.00738 | 0.87362 | 0.87875 |
| 85 | 1.09914 | -0.23356 | 0.00873 | 0.85686 | 0.86312 |
| 90 | 1.10921 | -0.26019 | 0.01006 | 0.83896 | 0.84654 |
| 92 | 1.11313 | -0.27109 | 0.01057 | 0.83148 | 0.83964 |
| 95 | 1.11880 | -0.28765 | 0.01127 | 0.81988 | 0.82901 |
| 100 | 1.12736 | -0.31561 | 0.01224 | 0.79951 | 0.81054 |